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13. ABSTRACT *(Maximum 200 words)*

Although the advent of fast and inexpensive parallel computers has rendered numerous previously intractable calculations feasible, many numerical simulations remain too resource intensive to be directly inserted into engineering optimization efforts. An alternative to direct insertion considers models for computational systems: the expensive simulation is evoked only to construct and validate a simplified input-output model; this simplified input-output model then serves as a simulation surrogate in subsequent engineering optimization studies. As compared to the direct insertion approach, surrogates offer more complete, efficient, and robust optimization, greater accommodation of prior information, broad applicability to families of objective functions, and a more interactive, flexible design environment.

In this project, a validated surrogate methodology was developed which permits economical and reliable integration of large-scale, possibly noisy numerical simulations into engineering design and optimization studies. The project included both the formulation, analysis, and implementation of construction-validations algorithms, and the application of the resulting techniques to problems of scientific and engineering interest. The sample application are intended to be sufficiently simple to permit numerical experiment, yet sufficiently complex to properly stimulate, constrain, and demonstrate the proposed methodology.

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FINAL REPORT

AFOSR Grant F49620-94-1-0121

"New Concepts in Computer Simulation-Surrogates"

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OVERVIEW

Although the advent of fast and inexpensive parallel computers has rendered numerous previously intractable calculations feasible, many numerical simulations remain too resource-intensive to be directly inserted into engineering optimization efforts. An attractive alternative to "direct insertion" considers models for computational systems: the expensive simulation is evoked only to construct and validate a simplified input-output model; this simplified input-output model then serves as a simulation surrogate in subsequent engineering optimization studies. As compared to the direct-insertion approach, surrogates offer more complete, efficient, and robust optimization, greater accommodation of prior information, broad applicability to families of objective functions, and a more interactive, flexible design environment.

In this project we have developed a validated surrogate methodology which permits economical and reliable integration of large-scale (possibly noisy) numerical simulations into engineering design and optimization studies. The project includes both the formulation, analysis, and implementation of construction-validation algorithms, and the application of the resulting techniques to problems of scientific and engineering interest. The sample applications are intended to be sufficiently simple to permit numerical experiment, yet sufficiently complex to properly stimulate, constrain, and demonstrate the proposed methodology.

Finally, we have interacted with United Technologies Research Center (UTRC) in two small grants which "leveraged" the AFOSR funding. The first grant, involving the integration of our methods into the UTRC simulation-based optimal design program, led to the application of our methods to certain problems of interest to Pratt and Whitney. The second grant focused on the particular issue of the effect of manufacturing tolerances on simulation-based design predictions.

TECHNICAL ACCOMPLISHMENTS

1. Basis Framework. The basic notions of construction, validation, and a *posteriori* error analysis are described in [1], with extension to the case of noisy outputs in [2]. The essential element of the framework is a nonparametric validation procedure that leads to a "probably approximately correct" error statement which then serves in the a *posteriori* analysis to estimate system predictability, optimality, and stability.

2. Algorithmic Improvements and Extensions. The basic techniques have been enhanced to permit: unbiased comparison and selection of competing candidate surrogates; elemental cross-validation procedures that permit the same simulation result to serve in both construction and validation; sequential validation techniques that permit construction and validation simulations to be deployed only as necessary, eliminating overconstruction and underconstruction as sources of inefficiency and inaccuracy, respectively; and adaptive construction and validation procedures that, based on local error estimators and sequential concepts, permit simulation results to be deployed only where needed in the design space. In addition, we have developed several new approaches to input noise and stability, simpler optimality metrics, multipoint "nonparametric-average" error estimates, effective error scalings for multiple outputs, and nested validation schemes based on a hierarchy of models. These results are described in [3,4,5].

3. Identification of Critical Issues. Through the work described above, it has become clear that the most important remaining issue is the treatment of problems with many inputs -- a common situation in many industrial situations. We have identified certain new techniques which, as an ensemble, should significantly improve our capability to address such problems.

The first ingredient is a Pareto optimization framework which, based on rational engineering design criteria, identifies and focuses on an appropriate *lower-dimensional* subset of the entire design space. The method has been applied successfully to several problems in optimal control and shape optimization.

The second ingredient is better construction (approximation) techniques that can yield good models based on relatively little expensive-simulation data. Towards this end, we have initiated development of Proper-Orthogonal-Decomposition methods that should perform significantly better than simple input-output interpolant (or fitting) schemes. The essential point is that POD techniques are based on a low-dimensional *state space*, and are thus much better able to capture complex dynamics than techniques which do not exploit the underlying structure of the governing equations. POD techniques should thus offer much better accuracy with less data and fewer modes. Application to several simple problems has demonstrated this claim.

The third ingredient is a new error estimation technique that will significantly decrease the cost of validation by permitting expensive truth calculations to be replaced by inexpensive but accurate lower and upper bounds. The methodology is based upon concepts from partial-differential-equation a *posteriori* error analysis, extended to permit the consideration of realistic (e.g., linear-functional) outputs. At present only a limited number of problems can be treated by this method, but the technique is, in theory, quite general, and should find broad applicability.

The three new ingredients described above have been evaluated in certain simple contexts, but much work remains to extend the ideas so that they can be applied to the complex problems encountered in industrial engineering design and optimization. This is the topic of our renewal grant, recently awarded by AFOSR.

PUBLICATIONS

1. S. Yesilyurt and A.T. Patera, "Surrogates for Numerical Simulations; Optimization of Eddy-Promoter Heat Exchangers," *Computer Methods in Applied Mechanics and Engineering*, 121 (1995), pp. 231-257.

2. S. Yesilyurt, C. Ghaddar, M.E. Cruz, and A.T. Patera, "Bayesian-Validated Surrogates for Noisy Computer Simulations; Application to Random Media," *SIAM J. Scientific Computing*, 17 (1996), pp. 973-992.

3. J.C. Otto, M. Paraschivoiu, S. Yesilyurt, and A.T. Patera, "Bayesian-Validated Computer-Simulation Surrogates for Optimization and Design," in *Proceedimgs ICASE Workshop on Multidisciplinary Design Optimization*, ed. N. Alexandrov, SIAM, Philadelphia, to appear.

4. J.C. Otto, M. Paraschivoiu, S. Yesilyurt, and A.T. Patera, "Bayesian-Validated Computer-Simulation Surrogates for Optimization and Design: Error Estimates and Applications", *IMACS J. Applied Numerical Mathematics*, to appear.

5. S. Yesilyurt, M. Paraschivoiu. J.C. Otto, and A.T. Patera, "Computer-Simulation Response Surfaces: A Bayesian-Validated Approach", in Proceedings Computational Methods in Water Resources XI, eds. Aldama, Aparicio, Brebbia, Gray, Herrera, Pinder, Vol. 1, pp. 13-22, *Computational Mechanics Publications*, Southampton, *1996.*